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Monte Carlo Simulation for Magnetic Domain Wall Displacements in Magnetic Nano-Wires With Local Disorders

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The velocities of magnetic domain wall displacements during reversal magnetization in a nano-wire were simulated as a function of impurity and defect densities in the host spin lattice, by using Monte Carlo method. The magnetic domain wall displacement velocity was enhanced for the clusters with defects and it was suppressed for ones with impurities.

***Index Terms*—Magnetic domains, magnetization processes, magnetization reversal, Monte Carlo (MC) methods.**

I. Introduction

RECENTLY, many experimental studies on magnetic domain wall displacements (DWD) have been performed with various micro magnetic clusters of 10-nm order in size [1], [2]. These studies will be available to realize new high-density, high-speed magnetic memories and micro-magnetic devices. Recent research on micromagnetic simulations, on the other hand, tends to be focused on spin transfer analysis [3], [4]. These simulations mainly base on the Landau–Lifshitz–Gilbert (LLG) equation which assumes homogeneity of magnetic materials without atomic size disorders, such as point defects, and also deal with magnetic properties under a sufficiently low temperature. The effects of inhomogeneity in magnetic clusters, however, have not been investigated sufficiently, e.g., for the clusters with point defects or magnetic impurities with reference to the dynamic DWD.

The Monte Carlo (MC) method is one of useful and powerful methods to simulate magnetic process for magnetic clusters including complicated interaction such as different exchange interactions due to different elements and to introduce magnetic properties depending on temperature [5], [6]. We tried to study on the DWD behaviors in magnetic nano-wires with atomic size disorders by using MC method, especially for the dependence of DWD velocities. The simulation, although it is semi-classical, will be useful for the study of intrinsic magnetic properties of magnetic nano-clusters including atomic size defects or impurities at finite temperature.

II. Numerical Models on MC Method

A rectangular solids spin system composed of $5 \times 5 \times 150$ cells $(0 \leq \mathrm{x} \leq 4, 0 \leq \mathrm{y} \leq 4, 0 \leq \mathrm{z} \leq 149)$ standing for a nano-wire was prepared as a normal spin system without any local disorder. A following Hamiltonian was used for the simulation:

$$\begin{aligned} H &= H_J + H_D + H_B \\ &= -\sum_{\text{near}} J_{ij}\mathbf{S}_i\mathbf{S}_j + D\sum_{\text{all}}\left(\frac{\mathbf{S}_i\cdot\mathbf{S}_j}{|\mathbf{r}_{ij}|^3}\right. \\ &\quad \left. -\frac{3}{|\mathbf{r}_{ij}|^5}(\mathbf{S}_i\cdot\mathbf{r}_{ij})(\mathbf{S}_j\cdot\mathbf{r}_{ij})\right) + B\sum_i \mathbf{S}_i. \end{aligned} \tag{1}$$

H_J term, H_D term, and H_B term represent exchange interaction energy, magnetic dipole interaction energy and applied magnetic field energy, respectively. Here, $\boldsymbol{S}_i$ denotes the magnetic moment of the spin state of ith cell and r_{ij} represents the vector between sites of ith spin and jth spin. Below we deal with clusters with the lattice constant of 1 and this is regarded as a criterion of length. In the first term, H_J, J_{ij} stands for an exchange interaction energy constant for ith and jth spins. Usually, exchange interaction works on only neighbor spins, because the interaction is originally due to overlapping between wave functions of electrons with spins, then the summation is limited to the extent in an effective radius r_{eff} from an original spin $\boldsymbol{S}_i$: $r_{ij} \leq r_{\text{eff}}$. In the second term, H_D, D stands for a magnetic dipole interaction constant. The magnetic dipole interaction works on all spins because it is due to magnetic field interspersed in all space. Then the summation includes the interaction energy between ith spin and all jth spins except for $j = i$. $\mathrm{H_D}$ forms the shape magnetic anisotropy with the easy axis along the longitudinal direction (z direction) for above spin system. In the third term H_B, B represents applied magnetic field which acts equally all spins. The changing of $\boldsymbol{S}_i$ on MC simulation progresses as spin-flips by Metropolis sampling at finite temperature $\mathrm{k_BT}$ [7], [8]. The period that N times of the spin-flips occur is called 1 MC step (MCS) for the cluster cell number N (=3750 in this case) and it corresponds to time passage in this simulation. For details of MC method for magnetic dynamic process, see the [9] and [10]. In this simulation, the parameters were set as $J_{ij} = 1.0$ between normal spins, $r_{\text{eff}} = 1.0, D = 0.1$. The value of $\boldsymbol{S}_i$ was fixed as $|\boldsymbol{S}_i| = 1$.

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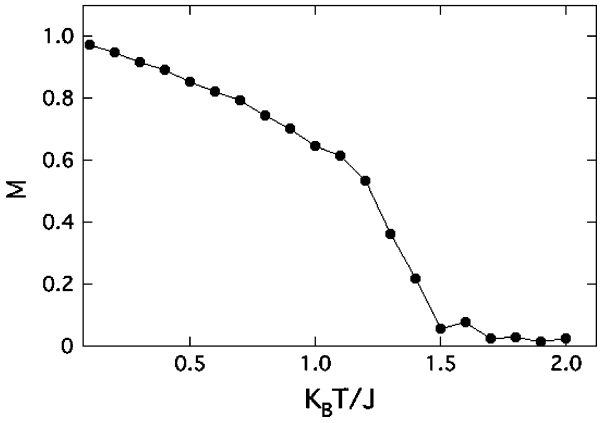

Fig. 1. Temperature dependence of normalized magnetization M for the rectangular cluster composed of $5 \times 5 \times 150$ spins. M was simulated cooling down from higher temperatures.

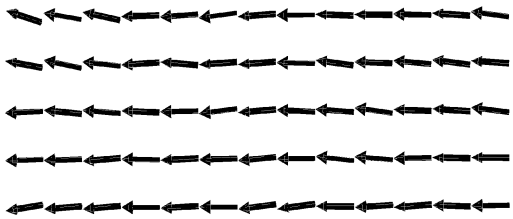

Fig. 2. Snapshot of the spin structure for the left edge of the rectangular cluster at the lowest temperature.

III. Results and Discussion

Fig. 1 shows temperature dependence of normalized magnetization M gradually cooling down from $\mathrm{k_BT} = 2.0$ to $\mathrm{k_BT} = 0.01$ for the rectangular cluster whose initial spin states were taken as random directions. Here, M is defined as follows:

$$M = \frac{1}{N}\left|\sum_i \mathbf{S}_i\right|. \tag{2}$$

At each temperature, M is determined after N MCS repeating for producing the results in equilibrium. The curve obeys the Curie Weiss law and it has the Curie temperature of about $\mathrm{k_BT_C} = 1.5$. At the lowest temperature, almost spins align toward the longitudinal direction of the rectangular cluster due to the shape magnetic anisotropy by magnetic dipole interaction between spins as shown in Fig. 2. Fig. 3 shows applied magnetic field dependence of normalized magnetization M_Z, that is, magnetic hysteresis curve. The direction of magnetic field B is set to the axis of z and applied on the process $B = 0^{\rightarrow} + 1.0^{\rightarrow} - 1.0^{\rightarrow} + 1.0$ with the step width $\Delta B = 0.01$. Here, M_Z is defined as follows:

$$M_z = \frac{1}{N}\sum_i \mathbf{S}_i \cdot \mathbf{k} \tag{3}$$

here, $\mathbf{k}$ is the unit vector along z-axis. The rectangular cluster has a large coecive force which would be due to the shape magnetic anisotropy. M_Z is saturated under the magnetic field of $B = 0.5$.

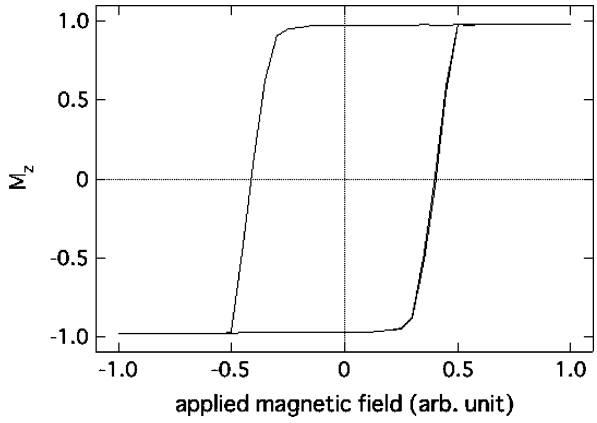

Fig. 3. Applied magnetic field dependence of M_Z (hysiteresis curve) for the rectangular cluster with $M_Z = -1.0$ at initial state.

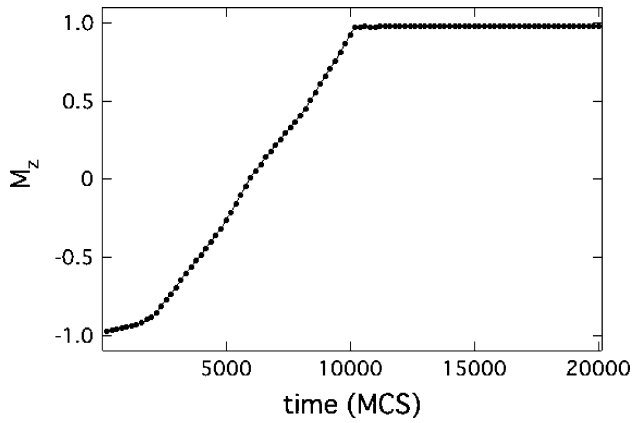

Fig. 4. Time dependence of M_Z under the constant reversal magnetic field of $B = +0.5$ for the rectangular cluster with $M_Z = -1.0$.

Next, the constant reversal magnetic field of $B = +0.5$ was applied for the rectangular cluster with $M_Z = -1.0$ at the lowest temperature in Fig. 1. Fig. 4 shows the time dependence of M_Z until 20000 MCS. The changing of M_Z is small until 2500 MCS, and M_Z changes with the almost constant gradient from 2500 MCS to 10000 MCS. Then M_Z becomes constant over 10000 MCS, that is, saturation magnetization. The period until 2500 MCS is an initial step of the reversal magnetization process that spin directions were first reversed from sites around both longitudinal edge sides ($\mathrm{z} = 0$ and 149) but obvious DWs are not produced yet. In the second period between 2500 and 10000 MCS, double DWs are produced around double edges of the rectangular cluster, as shown in Fig. 5(a), which shows a snapshot of the spin structure at $\mathrm{t} = 3000$ MCS. In the snapshot, there are double DWs at around $\mathrm{z} = 10$ and $\mathrm{z} = 140$ and the spins in the DWs take a screw structure, do not take Bloch or Neel typed DWs, as shown in Fig. 5(b).

These DWs run toward the middle of the cluster until 10000 MCS as shown in Fig. 6. In this figure, each line shows an average of absolute value of the z component of spins $(=\mathrm{S_z})$ included on the $\mathrm{x} - \mathrm{y}$ plane at each z position at each increasing time elapse. Then each dip on line corresponds to the DW position, because $\mathrm{S_z}$ becomes smaller around DW than ones in

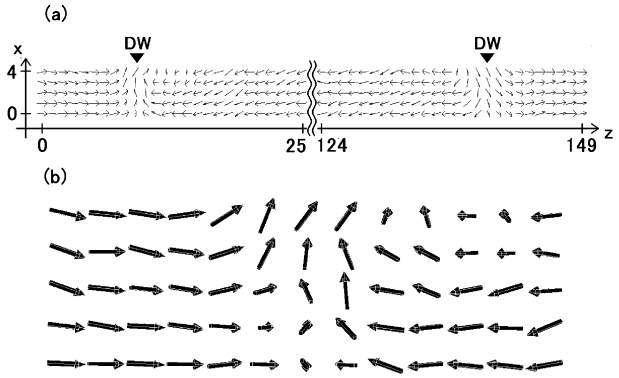

Fig. 5. (a) Snapshot of the spin structure during reversal magnetic field for the rectangular cluster at $t = 3000$ MCS after the magnetic field was applied. (b) Enlarged view of snapshot of the spin structure around the left side DW in (a).

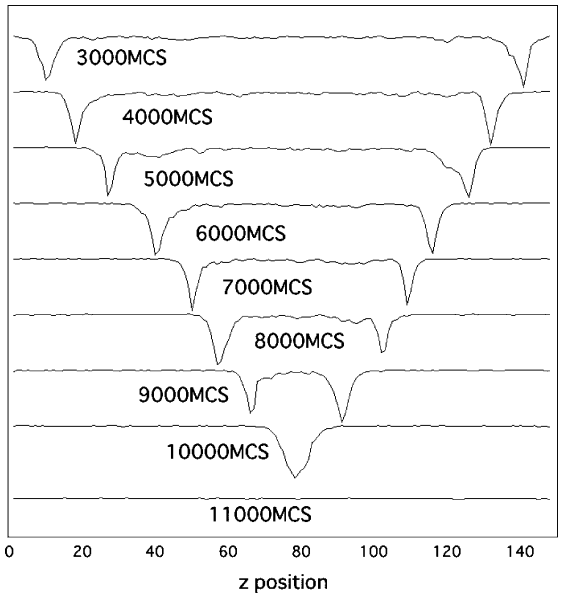

Fig. 6. Average of absolute value of S_z at each z position at each increasing time elapse, respectively. Each dip shows the DW position.

other positions. In the last step, the double DWs vanish after encounter each other around the middle of the rectangular cluster over 10000 MCS.

Fig. 7 shows the DW position depending on time elapses. In this model, using gradients of the DW position line for time, the DWD velocity was estimated as 0.93×10^{-2} (cell/MCS) for the rectangular cluster without defects or impurities. Note that the velocity cannot be estimated by M_Z in Fig. 3, because the rectangular cluster has double DW on reversal magnetization process and the increasing of M_Z is the result that the effects of double DWDs are superposed.

Here, atomic size disorders by magnetic impurities or point defects are introduced into the rectangular cluster as a normal spin system. These local disorders are randomly spread over the rectangular cluster until the number corresponding to the densities. Introducing of magnetic impurities is supposed to change no parameters of normal spins except for exchange interaction J_{ij}. The exchange interactions is set as $J_{ij} = 1.5$ between a normal spin and an impurity, and $J_{ij} = 2.0$ between impurities

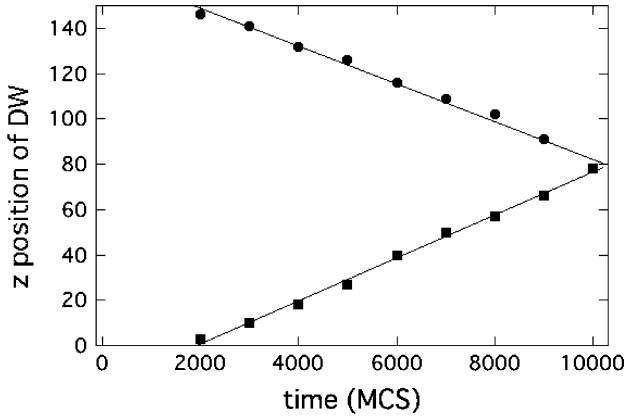

Fig. 7. Time dependence of the DW position on the left side (square markers) and right side (circle markers) of the rectangular cluster.

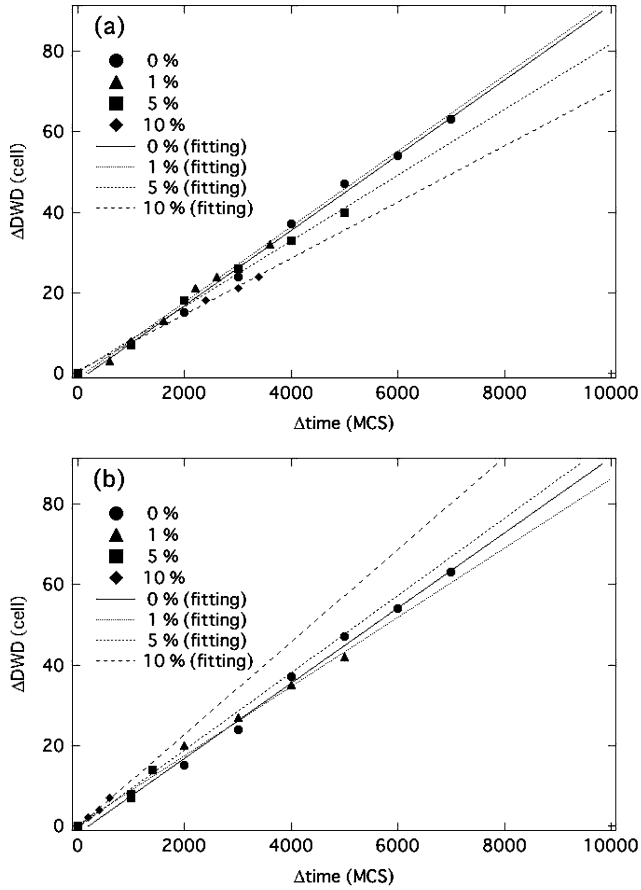

Fig. 8. Time dependence of the DW position changes of the rectangular cluster with various densities of (a) magnetic impurities and (b) defects.

expecting magnetic enhancement due to the impurity. Any interactions between a normal spin and a point defect or between point defects are set as zero because exchange interaction, magnetic dipole interaction and magnetic field do not act for a point defect which has no spins.

Fig. 8(a) shows time dependence of DW position changes (ΔDWD) for the rectangular cluster with magnetic impurities, since obvious DW is produced under the reversal magnetic field. It is clearly seen that the gradients decrease with increasing the density of impurities. On the other hand, the changes of

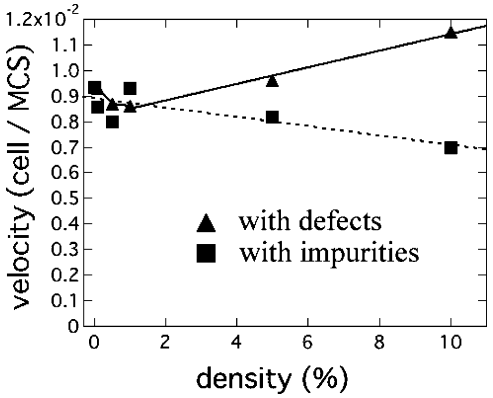

Fig. 9. DWD velocity changes with defect densities and impurity densities, respectively.

ΔDWDs per time for point defects are not obvious exactly as shown in Fig. 8(b), because in process of time, double DWs cannot keep themselves but many other DWs are produced until saturation magnetization, especially for the cluster with high density of point defects. Then the fitting lines of ΔDWDs per time for the cluster including over 5% densities of defects are calculated only for the beginning of ΔDWDs under 2000 MCS.

Fig. 9 shows variations of DWD velocity depending on magnetic impurities and point defects density. DWD velocity was found to decrease with increasing impurity. The stronger exchange interaction of impurity will act on DWD as a damping force. On the other hand DWD velocity increases with increasing point defect density, although it slightly decreases in the low density until 1%. Although usually it is thought that defects prevent magnetic domain wall from moving, the result that introducing defects enhance the DVD velocity, might be due to the large ratio of the defect density to the amount of all spins of the nano-cluster.

IV. Conclusion

DWD velocities were estimated for the rectangular clusters with different densities of magnetic impurities and defects by MC simulation. The method above mentioned for investigating the behavior of DW will be useful for the development of nano-magnetic devices in near future.

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